Abstract

Molecular docking study was performed on a series of 24 Thiazolidinediones MM1-MM24 as potential epiderma1 growth factor receptor (EGFR) inhibitors. The docking technique was applied to dock a set of representative compounds within the active site region of 1M17 using Molegro Virtual Docker v 5.0. For these compounds, the binding free energy (kcal/mol) was determined. The docking simulation clearly predicted the binding mode that is nearly similar to the crystallographic binding mode with 1.34Åo RMSD. Based on the validations and hydrogen bond interactions made by R substituents were considered for evaluation. The results avail to understand the type of interactions that occur between thiazolidinediones with 1M17 binding site region and explain the importance of R substitution on thiazolidinedione basic nucleus.

References

- Vasudeva Rao Avupati, Purna Nagasree Kurre, Santoshi Rupu Bagadi, Muralikrishna


**Index Terms**

Computer Science  
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**Keywords**

Molecular Docking  Thiazolidinediones  Epidermal growth factor receptor (EGFR)  Molegro Virtual Docker (MVD).